Author Index to Volume 148

Agmon, N., see S. Rabinovich 148 (1990) 11
Alonso, J.L., see J.C. López 148 (1990) 21

Bacci, M. and S. Cannistraro, Role of vibronic coupling for the temperature dependence of the *g*-tensor in proteins containing trigonal copper(II) ions 148 (1990) 451
Badawi, H.M., see J.R. Durig 148 (1990) 193
Bauder, A., see L. Martinache 148 (1990) 129
Bauschlicher Jr., C.W., H. Partridge and S.R. Langhoff, An ab initio study of the low-lying doublet states of AgO and AgS 148 (1990) 57
Beidoun, A., see A.V. Deshpande 148 (1990) 141
Beppu, Y. and T. Kakitani, Comprehensive study of molecular conformation and adiabatic potential surface of all-trans retinal by the CNDO/2 method 148 (1990) 333
Berger, H., see M.L. Gonze 148 (1990) 417
Bertrán, J., see E. Bosch 148 (1990) 77
Bonamy, J., see M.L. Gonze 148 (1990) 417
Bonamy, L., see M.L. Gonze 148 (1990) 417
Bosch, E., M. Moreno, J.M. Lluch and J. Bertrán, Comparison between intramolecular proton transfers involving the carboxylate and alkoxide groups 148 (1990) 77
Bott, J.F., R.F. Heidner, J.S. Holloway and J.B. Koffend, Photodissociation of XeF_2 at 193 nm 148 (1990) 411
Brion, C.E., see E.B. Zarate 148 (1990) 277
Brion, C.E., see E.B. Zarate 148 (1990) 289
Broo, A. and S. Larsson, Electron transfer due to through-bond interactions. Study of aliphatic chains 148 (1990) 103
Buchachenko, A.A., A.V. Nemukhin and N.F. Stepanov, Fragment-localized analysis of the multiconfigurational wavefunctions 148 (1990) 309

Cannistraro, S., see M. Bacci 148 (1990) 451
Cartier, C., see C. Mehadji 148 (1990) 95
Casarin, M., G. Granozzi, E. Tondello and A. Vittadini, A molecular cluster approach to the electronic structure of anomalous muonium in diamond 148 (1990) 183
Chaux, R., see M.L. Gonze 148 (1990) 417
Chermette, H., see C. Mehadji 148 (1990) 95
Chikkur, G.C., see S.M. Hanagodimath 148 (1990) 347
Clary, D.C., see G.-J. Kroes 148 (1990) 359
Cooper, G., see E.B. Zarate 148 (1990) 277
Cooper, G., see E.B. Zarate 148 (1990) 289

Daudey, J.-P., see M. Merchan 148 (1990) 69
Deshpande, A.V., A. Beidoun, A. Penzkofer and G. Wagenblast, Spectroscopic investigation of cyanovinyl-diethylaniline dyes in solutions 148 (1990) 141

Dolg, M., H. Stoll and H. Preuss, Ab initio pseudopotential study of europium monoxide EuO: $^8\Sigma^-$ ground state and $^8\Sigma^-$ first excited state 148 (1990) 219
Donovan, R.J., see T. Ridley 148 (1990) 315
Duguay, B., see T. Stoecklin 148 (1990) 381
Duguay, B., see T. Stoecklin 148 (1990) 399
Durig, J.R. and H.M. Badawi, Spectra and structure of small ring molecules. XLV. Microwave, infrared, and Raman spectra, conformational stability, dipole moment and vibrational assignment of cyclobutylcarboxaldehyde 148 (1990) 193

Fainberg, B.D., Non-linear polarization and spectroscopy of vibronic transitions in the field of intensive ultrashort pulses 148 (1990) 33
Ferretti, A. and A. Lami, Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation 148 (1990) 1

Gadaginamath, G.S., see S.M. Hanagodimath 148 (1990) 347
Gonzalez-Luque, R., see M. Merchan 148 (1990) 69
Gonze, M.L., R. Saint-Loup, J. Santos, B. Lavorel, R. Chaux, G. Millot, H. Berger, L. Bonamy, J. Bonamy and D. Robert, Collisional line broadening and line shifting in N_2–CO_2 mixture studied by inverse Raman spectroscopy 148 (1990) 417
Granozzi, G., see M. Casarin 148 (1990) 183

Hanagodimath, S.M., G.C. Chikkur and G.S. Gadaginamath, Environmental effects on the energy migration coefficient, the effective energy transfer and quenching distances in an organic liquid scintillator 148 (1990) 347
Hayes, M.A., see D.M.P. Holland 148 (1990) 241
Heidner, R.F., see J.F. Bott 148 (1990) 411
Herman, M.F. and C.E. Martinez, Approximate scaling relationships for exciton migration with trapping 148 (1990) 85
Hillier, I.H., see S.A. Jarrett-Sprague 148 (1990) 325
Holland, D.M.P., J.B. West and M.A. Hayes, The effect of autoionization on the Co_2^+ $X^2\Pi_g$ vibrational branching ratios in the wavelength range 680–790 Å 148 (1990) 241
Holloway, J.S., see J.F. Bott 148 (1990) 411

Itoh, N., see J. Singh 148 (1990) 209

Jarrett-Sprague, S.A. and I.H. Hillier, Ab initio calculations of the structure and infrared spectrum of As_2O and As_4O 148 (1990) 325

Kakitani, T., see Y. Beppu 148 (1990) 333
Karbach, H.-J., see B. Nickel 148 (1990) 155
Koffend, J.B., see J.F. Bott 148 (1990) 411
Koput, J., Ab initio study of the molecular structure and potential energy surface of disiloxane 148 (1990) 299
Krausz, E.R., see M.J. Riley 148 (1990) 229
Kresa, W., see L. Martinache 148 (1990) 129
Kroes, G.-J., R.P.H. Rettschnick and D.C. Clary, Rotationally and vibrationally inelastic scattering of glyoxal by helium at an energy of 96 meV 148 (1990) 359

Lami, A., see A. Ferretti 148 (1990) 1
Langhoff, S.R., see C.W. Bauschlicher Jr. 148 (1990) 57
Larsson, S., see A. Broo 148 (1990) 103
Lavorel, B., see M.L. Gonze 148 (1990) 417
Lawley, K.P., see T. Ridley 148 (1990) 315
Lesarri, A.G., see J.C. López 148 (1990) 21
Lister, D.G., see J.C. López 148 (1990) 21
Lluch, J.M., see E. Bosch 148 (1990) 77
López, J.C., A.G. Lesarri, D.G. Lister, J.L. Alonso, R.A. Shaw and H. Wieser, The microwave spectrum and ring-puckering vibration of 3-methyloxetane 148 (1990) 21

Martinache, L., W. Kresa, M. Wegener, U. Vonmont and A. Bauder, Microwave spectra and partial substitution structure of carboxylic acid bimolecules 148 (1990) 129
Martinez, C.E., see M.F. Herman 148 (1990) 85
Mehadji, C., S. Nour, H. Chermette, C. Cartier, S. Menage and M. Verdaguer, X-ray absorption of tetraoxomanganates (MnO_4^{n-}): experimental and MS LSD computational studies 148 (1990) 95
Menage, S., see C. Mehadji 148 (1990) 95
Merchan, M., J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil, On the dissociation energy of Cu_2 and CuH using a differential correlation approach 148 (1990) 69
Millot, G., see M.L. Gonze 148 (1990) 417
Moreno, M., see E. Bosch 148 (1990) 77

Nebot-Gil, I., see M. Merchan 148 (1990) 69
Nemukhin, A.V., see A.A. Buchachenko 148 (1990) 309
Ness, K.F. and L.A. Viehland, Distribution functions and transport coefficients for atomic ions in dilute gases 148 (1990) 255
Nickel, B. and H.-J. Karbach, Complete spectra of the delayed luminescence from aromatic compounds in liquid solutions; on the observability of direct radiative triplet–triplet annihilation 148 (1990) 155
Nour, S., see C. Mehadji 148 (1990) 95

Ortoleva, P. and R. Sultan, Static and propagating chemical spike structures and their electrical responses 148 (1990) 47

Partridge, H., see C.W. Bauschlicher Jr. 148 (1990) 57
Penzkofer, A., see A.V. Deshpande 148 (1990) 141
Preuss, H., see M. Dolg 148 (1990) 219

Rabinovich, S. and N. Agmon, The slow diffusion limit for the survival probability in reactive diffusion equations 148 (1990) 11
Rabitz, H., see M.J. Smith 148 (1990) 117
Rayez, J.C., see T. Stoecklin 148 (1990) 381
Rayez, J.C., see T. Stoecklin 148 (1990) 399
Rettschnick, R.P.H., see G.-J. Kroes 148 (1990) 359
Ridley, T., K.P. Lawley, R.J. Donovan and A.J. Yencha, Resonance enhanced (2+1) multiphoton ionization spectrum of Br_2: the lower Rydberg states 148 (1990) 315

Riley, M.J. and E.R. Krausz, The symmetric dimer: effects of second-order vibronic coupling 148 (1990) 229
Robert, D., see M.L. Gonze 148 (1990) 417

Saint-Loup, R., see M.L. Gonze 148 (1990) 417
Santos, J., see M.L. Gonze 148 (1990) 417
Shaw, R.A., see J.C. López 148 (1990) 21
Singh, J. and N. Itoh, A microscopic approach to the theory of polymer ablation 148 (1990) 209
Smith, M.J. and H. Rabitz, The connection between experimental observables and the potential energy surface in the He–HT system 148 (1990) 117
Stepanov, N.F., see A.A. Buchachenko 148 (1990) 309
Stoecklin, T., J.C. Rayez and B. Duguay, Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. III. Two analytic models of the lowest potential energy surface 148 (1990) 381
Stoecklin, T., J.C. Rayez and B. Duguay, Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. IV. A quasi-classical trajectory study of the reaction at 300 K 148 (1990) 399
Stoll, H., see M. Dolg 148 (1990) 219
Sultan, R., see P. Ortoleva 148 (1990) 47
Szubiakowski, J.P., Ground state transient linear dichroism for molecules with level-dependent rotational diffusion 148 (1990) 429

Tondello, E., see M. Casarin 148 (1990) 183

Verdaguer, M., see C. Mehadji 148 (1990) 95
Viehland, L.A., see K.F. Ness 148 (1990) 255
Vittadini, A., see M. Casarin 148 (1990) 183
Vonmont, U., see L. Martinache 148 (1990) 129

Wagenblast, G., see A.V. Deshpande 148 (1990) 141
Wallqvist, A., Incorporating intramolecular degrees of freedom in simulations of polarizable liquid water 148 (1990) 439
Wegener, M., see L. Martinache 148 (1990) 129
West, J.B., see D.M.P. Holland 148 (1990) 241
Wieser, H., see J.C. López 148 (1990) 21

Yencha, A.J., see T. Ridley 148 (1990) 315

Zarate, E.B., G. Cooper and C.E. Brion, Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. I. The valence shell 148 (1990) 277
Zarate, E.B., G. Cooper and C.E. Brion, Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. II. The P 2p and 2s inner shells 148 (1990) 289

List of Subjects

1 Methods

1.1 Theoretical

1.1.1 Group theory and algebras
1.1.2 Classical mechanics
1.1.3 Quantized field theory
1.1.4 Many body and quasiparticle approaches *
1.1.5 Coupling schemes and perturbative treatments *
1.1.6 Relativistic quantum mechanics *
1.1.7 Transport quantum mechanics *
1.1.8 Equilibrium statistical mechanics
1.1.9 Statistical mechanics of stationary states
1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories *
1.1.11 Ab initio schemes for stationary properties *
1.1.12 Computational and simulation methods *
1.1.13 Molecular dynamics and scattering theory *

1.2 Experimental

1.2.1 Magnetic resonances *
1.2.2 Cyclotron resonance
1.2.3 Microwave spectroscopy *
1.2.4 Infrared spectroscopy
1.2.5 Raman spectroscopy *
1.2.6 Visible and UV spectroscopy *
1.2.7 Fluorescence spectroscopy *
1.2.8 Photoelectron and Auger spectroscopy *
1.2.9 X-ray spectroscopy *
1.2.10 Electron impact spectroscopy
1.2.11 Laser methods *
1.2.12 Picosecond spectroscopy *
1.2.13 Non-linear optical spectroscopy
1.2.14 Synchrotron spectroscopies *
1.2.15 Coherent optical spectroscopy *
1.2.16 Optical pumping
1.2.17 Multiple resonance spectroscopy
1.2.18 Optoacoustic spectroscopy
1.2.19 Atomic and molecular beam techniques *
1.2.20 Time-resolved experiments *
1.2.21 Mass spectrometry
1.2.22 Radiolysis
1.2.23 Mössbauer spectroscopy
1.2.24 X-ray, electron and neutron diffraction
1.2.25 Neutron scattering
1.2.26 Light scattering
1.2.27 Field emission and field ionization
1.2.28 Measurement of macroscopic variables

2 Objects

2.1 Bulk systems

2.1.1 Gases *
2.1.2 Supersonic beams
2.1.3 Liquids neat *
2.1.4 Liquid mixtures and solutions *
2.1.5 Crystals *
2.1.5.1 neat *
2.1.5.2 mixed
2.1.6 Glasses
2.1.7 Liquid crystals
2.1.8 Polymers *
2.1.9 Semiconductors *
2.1.10 Metals and alloys
2.1.11 Thin films
2.1.12 Surfaces
2.1.13 Low-dimensional materials *
2.1.14 Dielectrics
2.1.15 Plasmas
2.1.16 Biological systems *

2.2 Microscopic systems

2.2.1 Atoms *
2.2.2 Molecules (neutral and ionic) *
2.2.2.1 diatomic *
2.2.2.2 small polyatomics *
2.2.2.3 aromatics *
2.2.2.4 other large
2.2.2.5 polymeric and biological *
2.2.3 Molecular aggregates *
2.2.3.1 dimers *
2.2.3.2 van der Waals molecules
2.2.3.3 clusters
2.2.3.4 complexes *
2.2.4 Free radicals (including hydronium and muonium)
2.2.5 Quasiparticles (including excitons) *
2.2.6 Defects and impurities *
2.2.7 Ions and charge carriers *

* Denotes subjects covered in this volume

3 Phenomena

3.1 Molecular structure *
3.2 Vibrations and rotations of molecules *
3.3 Electronic structure and states *
3.4 Electric and magnetic properties *
3.5 Spin splittings
3.6 Optical activity
3.7 Molecular interactions *
3.8 Spectral bandshapes and intensities *
3.9 Coupling of electronic and nuclear motion *
3.10 Energy transfer processes *
3.11 Molecular photophysical processes *
3.12 Intramolecular dynamics *
3.12.1 radiationless transitions
3.12.2 vibrational energy redistribution (including vibrational dissociation) *
3.13 Luminescence spectra, yields and lifetimes
3.14 Coherence loss processes
3.15 Non-linear responses (including optical) *
3.16 Multiphoton phenomena
3.17 Reactions (including dissociation) *
3.17.1 gas phase *
3.17.2 condensed phase
3.17.3 photochemical
3.18 Tunnelling *
3.19 Electron transfer *
3.20 Positron annihilation
3.21 Ionization (including Rydberg states)
3.22 Molecular motion (including diffusive) *
3.23 Isotopic effects
3.24 Fluctuations and noise
3.25 Collective motion and excitations *
3.26 Surface effects and catalysis
3.27 Thermodynamic and transport properties *
3.28 Structure of solids and liquids *
3.29 Critical phenomena
3.30 Phase transitions

Subject Index to Volume 148

Methods

Theoretical

Many body and quasiparticle approaches

Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation, A. Ferretti and A. Lami 148 (1990) 1
A microscopic approach to the theory of polymer ablation, J. Singh and N. Itoh 148 (1990) 209
Incorporating intramolecular degrees of freedom in simulations of polarizable liquid water, A. Wallqvist 148 (1990) 439

Coupling schemes and perturbative treatments

The slow diffusion limit for the survival probability in reactive diffusion equations, S. Rabinovich and N. Agmon 148 (1990) 11
The microwave spectrum and ring-puckering vibration of 3-methyloxetane, J.C. López, A.G. Lesarri, D.G. Lister, J.L. Alonso, R.A. Shaw and H. Wieser 148 (1990) 21
The symmetric dimer: effects of second-order vibronic coupling, M.J. Riley and E.R. Krausz 148 (1990) 229

Relativistic quantum mechanics

Ab initio pseudopotential study of europium monoxide EuO: $^8\Sigma^-$ ground state and $^8\Sigma^-$ first excited state, M. Dolg, H. Stoll and H. Preuss 148 (1990) 219

Transport quantum mechanics

Non-linear polarization and spectroscopy of vibronic transitions in the field of intensive ultrashort pulses, B.D. Fainberg 148 (1990) 33

Non-equilibrium thermodynamic and hydrodynamic theories

Static and propagating chemical spike structures and their electrical responses, P. Ortoleva and R. Sultan 148 (1990) 47

Ab initio schemes for stationary properties

An ab initio study of the low-lying doublet states of AgO and AgS, C.W. Bauschlicher Jr., H. Partridge and S.R. Langhoff 148 (1990) 57
On the dissociation energy of Cu_2 and CuH using a differential correlation approach, M. Merchan, J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil 148 (1990) 69
Comparison between intramolecular proton transfers involving the carboxylate and alkoxide groups, E. Bosch, M. Moreno, J.M. Lluch and J. Bertrán 148 (1990) 77
A molecular cluster approach to the electronic structure of anomalous muonium in diamond, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 148 (1990) 183

Ab initio pseudopotential study of europium monoxide EuO: $^8\Sigma^-$ ground state and $^8\Sigma^-$ first excited state, M. Dolg, H. Stoll and H. Preuss 148 (1990) 219
Ab initio study of the molecular structure and potential energy surface of disiloxane, J. Koput 148 (1990) 299
Ab initio calculations of the structure and infrared spectrum of As_2O and As_4O, S.A. Jarrett-Sprague and I.H. Hillier 148 (1990) 325

Computational and simulation methods
Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation, A. Ferretti and A. Lami 148 (1990) 1
Approximate scaling relationships for exciton migration with trapping, M.F. Herman and C.E. Martinez 148 (1990) 85
X-ray absorption of tetraoxomanganates (MnO_4^{n-}): experimental and MS LSD computational studies, C. Mehadji, S. Nour, H. Chermette, C. Cartier, S. Menage and M. Verdaguer 148 (1990) 95
Electron transfer due to through-bond interactions. Study of aliphatic chains, A. Broo and S. Larsson 148 (1990) 103
Distribution functions and transport coefficients for atomic ions in dilute gases, K.F. Ness and L.A. Viehland 148 (1990) 255
Fragment-localized analysis of the multiconfigurational wavefunctions, A.A. Buchachenko, A.V. Nemukhin and N.F. Stepanov 148 (1990) 309
Comprehensive study of molecular conformation and adiabatic potential surface of all-trans retinal by the CNDO/2 method, Y. Beppu and T. Kakitani 148 (1990) 333
Rotationally and vibrationally inelastic scattering of glyoxal by helium at an energy of 96 meV, G.-J. Kroes, R.P.H. Rettschnick and D.C. Clary 148 (1990) 359
Incorporating intramolecular degrees of freedom in simulations of polarizable liquid water, A. Wallqvist 148 (1990) 439

Molecular dynamics and scattering theory
The connection between experimental observables and the potential energy surface in the He–HT system, M.J. Smith and H. Rabitz 148 (1990) 117
Rotationally and vibrationally inelastic scattering of glyoxal by helium at an energy of 96 meV, G.-J. Kroes, R.P.H. Rettschnick and D.C. Clary 148 (1990) 359
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. III. Two analytic models of the lowest potential energy surface, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 381
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. IV. A quasi-classical trajectory study of the reaction at 300 K, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 399

Experimental

Magnetic resonances
Role of vibronic coupling for the temperature dependence of the *g*-tensor in proteins containing trigonal copper(II) ions, M. Bacci and S. Cannistraro 148 (1990) 451

Microwave spectroscopy
The microwave spectrum and ring-puckering vibration of 3-methyloxetane, J.C. López, A.G. Lesarri, D.G. Lister, J.L. Alonso, R.A. Shaw and H. Wieser 148 (1990) 21

Microwave spectra and partial substitution structure of carboxylic acid bimolecules, L. Martinache, W. Kresa, M. Wegener, U. Vonmont and A. Bauder 148 (1990) 129
Spectra and structure of small ring molecules. XLV. Microwave, infrared, and Raman spectra, conformational stability, dipole moment and vibrational assignment of cyclobutylcarboxaldehyde, J.R. Durig and H.M. Badawi 148 (1990) 193

Raman spectroscopy
Collisional line broadening and line shifting in N_2–CO_2 mixture studied by inverse Raman spectroscopy, M.L. Gonze, R. Saint-Loup, J. Santos, B. Lavorel, R. Chaux, G. Millot, H. Berger, L. Bonamy, J. Bonamy and D. Robert 148 (1990) 417

Visible and UV spectroscopy
Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. I. The valence shell, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 277
Photodissociation of XeF_2 at 193 nm, J.F. Bott, R.F. Heidner, J.S. Holloway and J.B. Koffend 148 (1990) 411

Fluorescence spectroscopy
Spectroscopic investigation of cyanovinyl-diethylaniline dyes in solutions, A.V. Deshpande, A. Beidoun, A. Penzkofer and G. Wagenblast 148 (1990) 141
Complete spectra of the delayed luminescence from aromatic compounds in liquid solutions; on the observability of direct radiative triplet–triplet annihilation, B. Nickel and H.-J. Karbach 148 (1990) 155
Environmental effects on the energy migration coefficient, the effective energy transfer and quenching distances in an organic liquid scintillator, S.M. Hanagodimath, G.C. Chikkur and G.S. Gadaginamath 148 (1990) 347

Photoelectron and Auger spectroscopy
The effect of autoionization on the CO_2^+ $X\,^2\Pi_g$ vibrational branching ratios in the wavelength range 680–790 Å, D.M.P. Holland, J.B. West and M.A. Hayes 148 (1990) 241

X-ray spectroscopy
X-ray absorption of tetraoxomanganates (MnO_4^{n-}): experimental and MS LSD computational studies, C. Mehadji, S. Nour, H. Chermette, C. Cartier, S. Menage and M. Verdaguer 148 (1990) 95
Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. II. The P 2p and 2s inner shells, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 289

Laser methods
Photodissociation of XeF_2 at 193 nm, J.F. Bott, R.F. Heidner, J.S. Holloway and J.B. Koffend 148 (1990) 411

Picosecond spectroscopy
Ground state transient linear dichroism for molecules with level-dependent rotational diffusion, J.P. Szubiakowski 148 (1990) 429

Synchrotron spectroscopies
X-ray absorption of tetraoxomanganates (MnO_4^{n-}): experimental and MS LSD computational studies, C. Mehadji, S. Nour, H. Chermette, C. Cartier, S. Menage and M. Verdaguer 148 (1990) 95
The effect of autoionization on the CO_2^+ $X^2\Pi_g$ vibrational branching ratios in the wavelength range 680–790 Å, D.M.P. Holland, J.B. West and M.A. Hayes 148 (1990) 241

Coherent optical spectroscopy
Resonance enhanced (2+1) multiphoton ionization spectrum of Br_2: the lower Rydberg states, T. Ridley, K.P. Lawley, R.J. Donovan and A.J. Yencha 148 (1990) 315

Atomic and molecular beam techniques
Microwave spectra and partial substitution structure of carboxylic acid bimolecules, L. Martinache, W. Kresa, M. Wegener, U. Vonmont and A. Bauder 148 (1990) 129

Time-resolved experiments
Non-linear polarization and spectroscopy of vibronic transitions in the field of intensive ultrashort pulses, B.D. Fainberg 148 (1990) 33
Ground state transient linear dichroism for molecules with level-dependent rotational diffusion, J.P. Szubiakowski 148 (1990) 429

Objects

Bulk systems

Gases
Spectra and structure of small ring molecules. XLV. Microwave, infrared, and Raman spectra, conformational stability, dipole moment and vibrational assignment of cyclobutylcarboxaldehyde, J.R. Durig and H.M. Badawi 148 (1990) 193
Distribution functions and transport coefficients for atomic ions in dilute gases, K.F. Ness and L.A. Viehland 148 (1990) 255
Resonance enhanced (2+1) multiphoton ionization spectrum of Br_2: the lower Rydberg states, T. Ridley, K.P. Lawley, R.J. Donovan and A.J. Yencha 148 (1990) 315
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. III. Two analytic models of the lowest potential energy surface, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 381
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. IV. A quasi-classical trajectory study of the reaction at 300 K, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 399
Collisional line broadening and line shifting in N_2–CO_2 mixture studied by inverse Raman spectroscopy, M.L. Gonze, R. Saint-Loup, J. Santos, B. Lavorel, R. Chaux, G. Millot, H. Berger, L. Bonamy, J. Bonamy and D. Robert 148 (1990) 417

Liquids neat
Incorporating intramolecular degrees of freedom in simulations of polarizable liquid water, A. Wallqvist 148 (1990) 439

Liquid mixtures and solutions
Complete spectra of the delayed luminescence from aromatic compounds in liquid solutions; on the observability of direct radiative triplet–triplet annihilation, B. Nickel and H.-J. Karbach 148 (1990) 155

Environmental effects on the energy migration coefficient, the effective energy transfer and quenching distances in an organic liquid scintillator, S.M. Hanagodimath, G.C. Chikkur and G.S. Gadaginamath 148 (1990) 347
Ground state transient linear dichroism for molecules with level-dependent rotational diffusion, J.P. Szubiakowski 148 (1990) 429

Crystals

–neat
Spectra and structure of small ring molecules. XLV. Microwave, infrared, and Raman spectra, conformational stability, dipole moment and vibrational assignment of cyclobutylcarboxaldehyde, J.R. Durig and H.M. Badawi 148 (1990) 193

Polymers
A microscopic approach to the theory of polymer ablation, J. Singh and N. Itoh 148 (1990) 209

Semiconductors
A molecular cluster approach to the electronic structure of anomalous muonium in diamond, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 148 (1990) 183

Low-dimensional materials
Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation, A. Ferretti and A. Lami 148 (1990) 1
Approximate scaling relationships for exciton migration with trapping, M.F. Herman and C.E. Martinez 148 (1990) 85

Biological systems
Comprehensive study of molecular conformation and adiabatic potential surface of all-trans retinal by the CNDO/2 method, Y. Beppu and T. Kakitani 148 (1990) 333
Role of vibronic coupling for the temperature dependence of the *g*-tensor in proteins containing trigonal copper(II) ions, M. Bacci and S. Cannistraro 148 (1990) 451

Microscopic systems

Atoms
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. III. Two analytic models of the lowest potential energy surface, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 381
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. IV. A quasi-classical trajectory study of the reaction at 300 K, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 399

Molecules (neutral and ionic)
Ab initio study of the molecular structure and potential energy surface of disiloxane, J. Koput 148 (1990) 299
Ground state transient linear dichroism for molecules with level-dependent rotational diffusion, J.P. Szubiakowski 148 (1990) 429

–diatomic

An ab initio study of the low-lying doublet states of AgO and AgS, C.W. Bauschlicher Jr., H. Partridge and S.R. Langhoff 148 (1990) 57

On the dissociation energy of Cu_2 and CuH using a differential correlation approach, M. Merchan, J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil 148 (1990) 69

Ab initio pseudopotential study of europium monoxide EuO: $^8\Sigma^-$ ground state and $^8\Sigma^-$ first excited state, M. Dolg, H. Stoll and H. Preuss 148 (1990) 219

Resonance enhanced (2+1) multiphoton ionization spectrum of Br_2: the lower Rydberg states, T. Ridley, K.P. Lawley, R.J. Donovan and A.J. Yencha 148 (1990) 315

Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. III. Two analytic models of the lowest potential energy surface, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 381

Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. IV. A quasi-classical trajectory study of the reaction at 300 K, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 399

–small polyatomics

Comparison between intramolecular proton transfers involving the carboxylate and alkoxide groups, E. Bosch, M. Moreno, J.M. Lluch and J. Bertrán 148 (1990) 77

X-ray absorption of tetraoxomanganates (MnO_4^{n-}): experimental and MS LSD computational studies, C. Mehadji, S. Nour, H. Chermette, C. Cartier, S. Menage and M. Verdaguer 148 (1990) 95

Spectra and structure of small ring molecules. XLV. Microwave, infrared, and Raman spectra, conformational stability, dipole moment and vibrational assignment of cyclobutylcarboxaldehyde, J.R. Durig and H.M. Badawi 148 (1990) 193

The effect of autoionization on the CO_2^+ $X^2\Pi_g$ vibrational branching ratios in the wavelength range 680–790 Å, D.M.P. Holland, J.B. West and M.A. Hayes 148 (1990) 241

Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. I. The valence shell, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 277

Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. II. The P 2p and 2s inner shells, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 289

Ab initio study of the molecular structure and potential energy surface of disiloxane, J. Koput 148 (1990) 299

Photodissociation of XeF_2 at 193 nm, J.F. Bott, R.F. Heidner, J.S. Holloway and J.B. Koffend 148 (1990) 411

–aromatics

Non-linear polarization and spectroscopy of vibronic transitions in the field of intensive ultrashort pulses, B.D. Fainberg 148 (1990) 33

Spectroscopic investigation of cyanovinyl-diethylaniline dyes in solutions, A.V. Deshpande, A. Beidoun, A. Penzkofer and G. Wagenblast 148 (1990) 141

Complete spectra of the delayed luminescence from aromatic compounds in liquid solutions; on the observability of direct radiative triplet–triplet annihilation, B. Nickel and H.-J. Karbach 148 (1990) 155

–polymeric and biological

Comprehensive study of molecular conformation and adiabatic potential surface of all-trans retinal by the CNDO/2 method, Y. Beppu and T. Kakitani 148 (1990) 333

Molecular aggregates

–dimers
The symmetric dimer: effects of second-order vibronic coupling, M.J. Riley and E.R. Krausz 148 (1990) 229

–complexes
Microwave spectra and partial substitution structure of carboxylic acid bimolecules, L. Martinache, W. Kresa, M. Wegener, U. Vonmont and A. Bauder 148 (1990) 129

Quasiparticles (including excitons)
Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation, A. Ferretti and A. Lami 148 (1990) 1
Approximate scaling relationships for exciton migration with trapping, M.F. Herman and C.E. Martinez 148 (1990) 85

Defects and impurities
A molecular cluster approach to the electronic structure of anomalous muonium in diamond, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 148 (1990) 183

Ions and charge carriers
Distribution functions and transport coefficients for atomic ions in dilute gases, K.F. Ness and L.A. Viehland 148 (1990) 255

Phenomena

Molecular structure
The microwave spectrum and ring-puckering vibration of 3-methyloxetane, J.C. López, A.G. Lesarri, D.G. Lister, J.L. Alonso, R.A. Shaw and H. Wieser 148 (1990) 21
On the dissociation energy of Cu_2 and CuH using a differential correlation approach, M. Merchan, J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil 148 (1990) 69
Microwave spectra and partial substitution structure of carboxylic acid bimolecules, L. Martinache, W. Kresa, M. Wegener, U. Vonmont and A. Bauder 148 (1990) 129
Spectroscopic investigation of cyanovinyl-diethylaniline dyes in solutions, A.V. Deshpande, A. Beidoun, A. Penzkofer and G. Wagenblast 148 (1990) 141
Spectra and structure of small ring molecules. XLV. Microwave, infrared, and Raman spectra, conformational stability, dipole moment and vibrational assignment of cyclobutylcarboxaldehyde, J.R. Durig and H.M. Badawi 148 (1990) 193
Ab initio pseudopotential study of europium monoxide EuO: $^8\Sigma^-$ ground state and $^8\Sigma^-$ first excited state, M. Dolg, H. Stoll and H. Preuss 148 (1990) 219
Ab initio study of the molecular structure and potential energy surface of disiloxane, J. Koput 148 (1990) 299
Ab initio calculations of the structure and infrared spectrum of As_2O and As_4O, S.A. Jarrett-Sprague and I.H. Hillier 148 (1990) 325
Comprehensive study of molecular conformation and adiabatic potential surface of all-trans retinal by the CNDO/2 method, Y. Beppu and T. Kakitani 148 (1990) 333

Vibrations and rotations of molecules
The microwave spectrum and ring-puckering vibration of 3-methyloxetane, J.C. López, A.G. Lesarri, D.G. Lister, J.L. Alonso, R.A. Shaw and H. Wieser 148 (1990) 21
The connection between experimental observables and the potential energy surface in the He–HT system, M.J. Smith and H. Rabitz 148 (1990) 117
Microwave spectra and partial substitution structure of carboxylic acid bimolecules, L. Martinache, W. Kresa, M. Wegener, U. Vonmont and A. Bauder 148 (1990) 129
Ab initio study of the molecular structure and potential energy surface of disiloxane, J. Koput 148 (1990) 299
Ab initio calculations of the structure and infrared spectrum of As_2O and As_4O, S.A. Jarrett-Sprague and I.H. Hillier 148 (1990) 325
Rotationally and vibrationally inelastic scattering of glyoxal by helium at an energy of 96 meV, G.-J. Kroes, R.P.H. Rettschnick and D.C. Clary 148 (1990) 359

Electronic structure and states
An ab initio study of the low-lying doublet states of AgO and AgS, C.W. Bauschlicher Jr., H. Partridge and S.R. Langhoff 148 (1990) 57
Spectroscopic investigation of cyanovinyl-diethylaniline dyes in solutions, A.V. Deshpande, A. Beidoun, A. Penzkofer and G. Wagenblast 148 (1990) 141
A molecular cluster approach to the electronic structure of anomalous muonium in diamond, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 148 (1990) 183
Ab initio pseudopotential study of europium monoxide EuO: $^8\Sigma^-$ ground state and $^8\Sigma^-$ first excited state, M. Dolg, H. Stoll and H. Preuss 148 (1990) 219
The symmetric dimer: effects of second-order vibronic coupling, M.J. Riley and E.R. Krausz 148 (1990) 229
Fragment-localized analysis of the multiconfigurational wavefunctions, A.A. Buchachenko, A.V. Nemukhin and N.F. Stepanov 148 (1990) 309
Resonance enhanced (2+1) multiphoton ionization spectrum of Br_2: the lower Rydberg states, T. Ridley, K.P. Lawley, R.J. Donovan and A.J. Yencha 148 (1990) 315
Comprehensive study of molecular conformation and adiabatic potential surface of all-trans retinal by the CNDO/2 method, Y. Beppu and T. Kakitani 148 (1990) 333

Electric and magnetic properties
Distribution functions and transport coefficients for atomic ions in dilute gases, K.F. Ness and L.A. Viehland 148 (1990) 255

Molecular interactions
The connection between experimental observables and the potential energy surface in the He–HT system, M.J. Smith and H. Rabitz 148 (1990) 117
Complete spectra of the delayed luminescence from aromatic compounds in liquid solutions; on the observability of direct radiative triplet–triplet annihilation, B. Nickel and H.-J. Karbach 148 (1990) 155
Fragment-localized analysis of the multiconfigurational wavefunctions, A.A. Buchachenko, A.V. Nemukhin and N.F. Stepanov 148 (1990) 309
Collisional line broadening and line shifting in N_2–CO_2 mixture studied by inverse Raman spectroscopy, M.L. Gonze, R. Saint-Loup, J. Santos, B. Lavorel, R. Chaux, G. Millot, H. Berger, L. Bonamy, J. Bonamy and D. Robert 148 (1990) 417
Incorporating intramolecular degrees of freedom in simulations of polarizable liquid water, A. Wallqvist 148 (1990) 439

Spectral bandshapes and intensities
X-ray absorption of tetraoxomanganates (MnO_4^{n-}): experimental and MS LSD computational studies, C. Mehadji, S. Nour, H. Chermette, C. Cartier, S. Menage and M. Verdaguer 148 (1990) 95
Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. I. The valence shell, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 277
Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. II. The P 2p and 2s inner shells, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 289
Collisional line broadening and line shifting in N_2–CO_2 mixture studied by inverse Raman spectroscopy, M.L. Gonze, R. Saint-Loup, J. Santos, B. Lavorel, R. Chaux, G. Millot, H. Berger, L. Bonamy, J. Bonamy and D. Robert 148 (1990) 417

Coupling of electronic and nuclear motion
The symmetric dimer: effects of second-order vibronic coupling, M.J. Riley and E.R. Krausz 148 (1990) 229
The effect of autoionization on the CO_2^+ $X\,^2\Pi_g$ vibrational branching ratios in the wavelength range 680–790 Å, D.M.P. Holland, J.B. West and M.A. Hayes 148 (1990) 241
Role of vibronic coupling for the temperature dependence of the *g*-tensor in proteins containing trigonal copper(II) ions, M. Bacci and S. Cannistraro 148 (1990) 451

Energy transfer processes
The connection between experimental observables and the potential energy surface in the He–HT system, M.J. Smith and H. Rabitz 148 (1990) 117
A microscopic approach to the theory of polymer ablation, J. Singh and N. Itoh 148 (1990) 209
Environmental effects on the energy migration coefficient, the effective energy transfer and quenching distances in an organic liquid scintillator, S.M. Hanagodimath, G.C. Chikkur and G.S. Gadaginamath 148 (1990) 347
Rotationally and vibrationally inelastic scattering of glyoxal by helium at an energy of 96 meV, G.-J. Kroes, R.P.H. Rettschnick and D.C. Clary 148 (1990) 359
Collisional line broadening and line shifting in N_2–CO_2 mixture studied by inverse Raman spectroscopy, M.L. Gonze, R. Saint-Loup, J. Santos, B. Lavorel, R. Chaux, G. Millot, H. Berger, L. Bonamy, J. Bonamy and D. Robert 148 (1990) 417

Molecular photophysical processes
Complete spectra of the delayed luminescence from aromatic compounds in liquid solutions; on the observability of direct radiative triplet–triplet annihilation, B. Nickel and H.-J. Karbach 148 (1990) 155
The effect of autoionization on the CO_2^+ $X\,^2\Pi_g$ vibrational branching ratios in the wavelength range 680–790 Å, D.M.P. Holland, J.B. West and M.A. Hayes 148 (1990) 241
Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. I. The valence shell, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 277
Absolute oscillator strengths for the photoabsorption, photoionization and ionic photofragmentation of phosphine. II. The P 2p and 2s inner shells, E.B. Zarate, G. Cooper and C.E. Brion 148 (1990) 289
Photodissociation of XeF_2 at 193 nm, J.F. Bott, R.F. Heidner, J.S. Holloway and J.B. Koffend 148 (1990) 411

Intramolecular dynamics
The microwave spectrum and ring-puckering vibration of 3-methyloxetane, J.C. López, A.G. Lesarri, D.G. Lister, J.L. Alonso, R.A. Shaw and H. Wieser 148 (1990) 21

–vibrational energy redistribution (including vibrational dissociation)
Non-linear polarization and spectroscopy of vibronic transitions in the field of intensive ultrashort pulses, B.D. Fainberg 148 (1990) 33

Non-linear responses (including optical)
Non-linear polarization and spectroscopy of vibronic transitions in the field of intensive ultrashort pulses, B.D. Fainberg 148 (1990) 33
Static and propagating chemical spike structures and their electrical responses, P. Ortoleva and R. Sultan 148 (1990) 47

Reactions (including dissociation)

–gas phase
Comparison between intramolecular proton transfers involving the carboxylate and alkoxide groups, E. Bosch, M. Moreno, J.M. Lluch and J. Bertrán 148 (1990) 77
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. III. Two analytic models of the lowest potential energy surface, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 381
Theoretical study of the reaction $C(^3P)+SH(X^2\Pi)$. IV. A quasi-classical trajectory study of the reaction at 300 K, T. Stoecklin, J.C. Rayez and B. Duguay 148 (1990) 399

Tunnelling
Electron transfer due to through-bond interactions. Study of aliphatic chains, A. Broo and S. Larsson 148 (1990) 103
The symmetric dimer: effects of second-order vibronic coupling, M.J. Riley and E.R. Krausz 148 (1990) 229

Electron transfer
Electron transfer due to through-bond interactions. Study of aliphatic chains, A. Broo and S. Larsson 148 (1990) 103

Molecular motion (including diffusive)
The slow diffusion limit for the survival probability in reactive diffusion equations, S. Rabinovich and N. Agmon 148 (1990) 11
Ground state transient linear dichroism for molecules with level-dependent rotational diffusion, J.P. Szubiakowski 148 (1990) 429

Collective motion and excitations
Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation, A. Ferretti and A. Lami 148 (1990) 1

Thermodynamic and transport properties
Static and propagating chemical spike structures and their electrical responses, P. Ortoleva and R. Sultan 148 (1990) 47
Distribution functions and transport coefficients for atomic ions in dilute gases, K.F. Ness and L.A. Viehland 148 (1990) 255

Structure of solids and liquids
Hole pairing on oxygen sites in high-T_c copper oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation, A. Ferretti and A. Lami 148 (1990) 1
Incorporating intramolecular degrees of freedom in simulations of polarizable liquid water, A. Wallqvist 148 (1990) 439